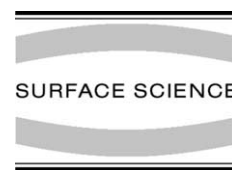




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5f Resonant photoemission from plutonium

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Abstract

Experimental resonant photoemission (ResPes) results for α -Pu and δ -Pu bulk samples are presented and compared to the results of an atomic model calculation. Both Pu samples exhibit limited agreement with the atomic model calculations. As expected, α -Pu appears to have more 5f valence band delocalization than δ -Pu. Evidence of an enhanced sensitivity to surface corruption, by using synchrotron radiation as the excitation, is presented. © 2001 Elsevier Science B.V. All rights reserved.

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The valence electronic structures of the actinide metals and alloys in general and plutonium (Pu) in particular remain mired in controversy [1–5]. Interestingly, the various phases of Pu metal provide a microcosm of the metallic actinides as a whole [6–9]. Thus, unravelling the nuances of the interplay of electronic and geometric structures in Pu will illuminate the properties of all transuranic metals. In a sense, the behavior of the Pu 5f elec-

trons is completely counter-intuitive. The dense phase, α , has some semblance of delocalization in the 5f valence bands and can be treated theoretically within single electron models such as the local density approximation (LDA). The α phase is monoclinic, which is a low symmetry ordering [10]. The less dense δ -phase is fcc and exhibits evidence of localized and/or correlated electronic behavior. The fcc is a high symmetry phase which is normally associated with superior wave function overlap in d state metals. But herein is the key: the linear combinations of the 5f's do not produce the nicely lobed wave functions with symmetry about the x , y , z and diagonal axes, as occurs for d states. Instead, the linear combinations of f-states have oddly lobed and badly directed wave functions

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